

On the geometry of quantum constrained systems

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Abstract

The use of geometric methods has proved useful in the hamiltonian description of classical constrained systems. Here we put forward the first steps toward the description of the geometry of *quantum* constrained systems. We make use of the geometric formulation of quantum theory in which unitary transformations (including time evolution) can be seen, just as in the classical case, as finite canonical transformations on the quantum state space. We compare from this perspective the classical and quantum formalisms and argue that there is an important difference between them, that suggests that the condition on observables to become *physical* is through the double commutator with the square of the constraint operator. This provides a bridge between the standard Dirac-Bergmann procedure –through its geometric implementation– and the *Master Constraint* program.

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I. INTRODUCTION

It is well known that most of the fundamental theories of physics, when analyzed from the hamiltonian perspective, are subject to constraints $C_i \approx 0$ between their canonical variables. Notable examples of these systems are totally constrained systems; theories whose Hamiltonian is a combination of constraints, and whose time evolution is therefore also governed by constraints, such as general relativity defined over a compact Cauchy surface. The description of classical constrained hamiltonian systems has benefited from the use of symplectic geometry. For instance, the classification into first and second class constraints by Dirac has a direct description in terms of the degeneracy properties of the symplectic two-form on the constrained surface. Like-wise, the gauge invariant information can be encoded in a geometric fashion by means of the quotient along gauge orbits of first class constraints [1, 2]. A natural question is whether one can extend this geometric understanding into the quantum description for constrained systems.

There are two main strategies for dealing with the canonical quantization of constrained systems; one can follow either the Dirac or the Reduced Phase Space (RPS) approach to quantization, and within each one, different implementation procedures are possible. For instance, in recent years, several methods for implementing the Dirac approach have been developed, such as the refined algebraic quantization (RAQ) [3] and coherent state quantization [4]. In particular, the RAQ method has been extremely successful in dealing with model systems in gravity and cosmology [2, 3, 4]. More recently, a *Master Constraint Program* has been put forward to deal with the quantization of constrained systems [5].

Here we will consider the quantization of systems subject to first class constraints within the so called Dirac-Bergmann approach. This means that the reduction of the degrees of freedom from the kinematical unconstrained theory to the physical constrained system is achieved by the imposition of quantum constraints on the states. The constraints are promoted to operators \hat{C}_i on the kinematical Hilbert space and the physical states are those for which the Dirac conditions

$$\hat{C}_i \cdot \Psi = 0$$

are satisfied. The first difference between the classical and quantum treatment is obvious. While in the classical theory the full gauge reduction is performed in two steps, in the quantum domain there is only one condition to be satisfied. As is well known, this only step in the quantum realm is the precise equivalent of the two step procedure of the classical domain.

The purpose of this note is to explore this quantum reduction from a geometrical perspective. The classical reduction is well known in terms of the symplectic geometry of the constrained surface $\bar{\Gamma} \subset \Gamma$. However, in its traditional formulation, the quantum reduction does not admit such an interpretation. In order to overcome this we shall consider the reduction from the perspective of the geometric formulation of quantum mechanics [7]. In this formulation, the quantum space of states \mathcal{P} formed out of rays in the Hilbert space \mathcal{H} , acquires the structure of a Kähler manifold endowed with both a symplectic structure responsible for the implementation of unitary transformations, and a Riemannian structure relevant for the uncertainties and probabilistic aspects of the quantum theory.

As we shall show, the Dirac quantum conditions, for the simplest case where the physical Hilbert space is a sub-vector space, can be cast in the same form as the classical conditions: as the inverse image of zero for some functions \mathcal{C}_i on the quantum state space \mathcal{P} . Thus, the

physical quantum state space $\mathcal{P}_{\text{phy}} \subset \mathcal{P}$ is also a submanifold of the total state space¹. One could perhaps expect that the induced geometry on the constrained surface be analogous to the classical case, with degenerate –gauge– directions. If this were the case, however, we would need to perform a second reduction along the ‘quantum gauge orbits’ which would be in contradiction with the fact that no further reduction is necessary. As we will see, there is indeed a simple justification of this procedure and a geometrical interpretation in terms of which this difference can be readily understood. More precisely, we will show that the detailed form of the functions that implement the constraint does not allow for this possibility. There are no further gauge orbits. Second, we consider the issue of observables, their characterization and algebraic properties. We show that the geometric formulation provides a new perspective on the issue of Dirac observables. Their natural geometric characterization provides a precise prescription that can be seen to coincide with the one given by the double commutator of the master constraint program [5].

The structure of this paper is as follows. In Sec. II we review the geometric treatment of classical mechanics, including a brief introduction to constrained systems. Readers familiar with this formalism may safely skip it. Sec. III is the main section of this paper and has two parts. In the first one, we recall the geometric formulation of quantum mechanics without constraints. In the second part we extend the formalism to consider constraints. We explore the algebra of constraints and the conditions for observables to be physical. We end with a brief discussion and outlook in Sec. IV. We have tried to make the article self-contained so only some familiarity with the symplectic formulation of mechanics is assumed.

II. CLASSICAL CONSTRAINED SYSTEMS

In this section we recall the usual treatment of constrained hamiltonian systems from the perspective of the underlying symplectic geometry. We shall not review the Dirac-Bergmann procedure in order to arrive at the final hamiltonian picture, but instead assume that the hamiltonian system (together with its constraints) has been given to us. For a detailed account of the Dirac procedure see [2] and [6].

A physical system is normally represented, at the classical hamiltonian level, by a *phase space*, consisting of a manifold Γ of even dimension $2N$. The symplectic two-form Ω endows it with the structure of a symplectic space (Γ, Ω) . A vector field V^a generates infinitesimal canonical transformations if it Lie drags the symplectic form, i.e.:

$$\mathcal{L}_V \Omega = 0 \tag{1}$$

This condition is equivalent to saying that, locally, the symplectic form satisfies: $V^b = \Omega^{ba} \nabla_a f := X_f^b$, for some function f . The vector X_f^a is called the *Hamiltonian vector field (HVF)* of f (*w.r.t.* Ω). Note that the non-degenerate symplectic structure Ω gives us a mapping between functions on Γ and Hamiltonian vector fields. Thus, functions on phase space, i.e. observables, are generators of infinitesimal canonical transformations.

The Lie Algebra of vector fields induces a Lie Algebra structure $\{\cdot, \cdot\}$, the *Poisson Bracket* (PB) on the space of functions,

$$\{f, g\} := \Omega_{ab} X_g^a X_f^b = \Omega^{ab} \nabla_a f \nabla_b g \tag{2}$$

¹ In Ref. [8] the application of geometric methods to gauge systems was also explored, but from a slightly different perspective, using techniques from BRST.

such that $X_{\{f,g\}}^a = -[X_f, X_g]^a$. The Poisson bracket $\{f, g\}$ gives the change of f given by the motion generated by (the HVF of) g , i.e.,

$$\{f, g\} = \mathcal{L}_{X_g} f \quad (3)$$

The PB is antisymmetric so it also gives (minus) the change of g generated by f .

When the physical system under consideration has constraints, these are manifested through M constraint functions $C_i : \Gamma \rightarrow \mathbb{R}$ relating the phase space variables. A point $p \in \Gamma$ belongs to the constraint surface $\bar{\Gamma}$ iff $C_i(p) = 0$ for all $i = 1, 2, \dots, M$. That is, the constraint surface $\bar{\Gamma}$ is the intersection of the M codimension-one surfaces defined by the vanishing of each of the constraint functions. If the resulting subspace is a manifold and the gradients $\nabla_a C_i$ of all the constraint functions are independent and non-vanishing on $\bar{\Gamma}$, then the constraint functions represent an ‘admissible description’ of the $(2N-M)$ -dimensional constraint surface $\bar{\Gamma}$. We shall only consider the case in which the set C_i forms a *first class system*. This means that, under Poisson brackets, they satisfy:

$$\{C_i, C_j\} = F_{ij}^k C_k \quad (4)$$

for some structure functions F_{ij}^k (i.e. phase space dependent quantities). Given that this relation can be translated to the corresponding HVF, this means that the M vector fields $X_i^a := \Omega^{ab} \nabla_b C_i$ are, at each point of $\bar{\Gamma}$, closed under the commutator. Furthermore, the condition (4) also implies that all the HVF’s X_i^a are tangent to $\bar{\Gamma}$ (and integrable). Even more, X_i^a represent the *degenerate* directions of the two form $\bar{\Omega}$, the restriction of Ω to $\bar{\Gamma}$:

$$\bar{V}^a \Omega_{ab} X_i^a = -\bar{V}^a \nabla_a C_i = 0 \quad (5)$$

for all \bar{V}^a tangent to $\bar{\Gamma}$ and all i .

The standard ‘Dirac conjecture’ states that the points along the orbits of the constraint vector fields represent physically indistinguishable configurations and are thus regarded as *gauge* [2, 6]. Those orbits are sometimes called the gauge orbits. The fact that the vector fields are integrable allows one to define an equivalence class $[p]$ of points that lie on the same gauge orbit. Furthermore, one can take the quotient by the orbits and the resulting space (if it is a manifold) is the reduced phase space $\hat{\Gamma}$. A point there represent a ‘physical state’ of the system. This is precisely the classical two step process consisting of restriction to the constraint surface and then quotient by the gauge orbits. As we show now, this ‘conjecture’ is completely justified from the geometric perspective.

Let us now consider observables. It is clear that not every function f on the phase space Γ will be an observable, since classically one is restricted to the constraint surface to begin with. This means that one only has direct access to the restriction of the function f to the space $\bar{\Gamma}$, so the information contained by the function off the surface is irrelevant. Let us then assume that we only consider functions from $\bar{\Gamma}$ to the real numbers. Is any such function an observable? The answer is no.

One should expect that physical observables are such that they preserve the defining properties of the system. That is, the observables as generators of finite canonical transformations (symplectomorphisms) should be such that they leave the constraint surface invariant. We shall take this as a definition and examine what this implies when considering the Poisson bracket:

$$0 = \{C_i, f\} = X_f^a \nabla_a C_i = -X_i^a \nabla_a f \quad (6)$$

That is, an observable is such that its HVF (and its integral curve) is tangent to $\bar{\Gamma}$. This means that the finite symplectic transformations generated by the observables preserve the constraint surface, as one should require. If one considers a function defined everywhere on Γ with the property that its HVF (when restricted to $\bar{\Gamma}$) is tangent to the constraint surface then it is called a *weak* observable. If the condition (6) is valid everywhere on Γ it is called a *strong* observable. This last condition seems to be too strong and unnecessary given that whatever happens outside the constraint surface is rather irrelevant for the system, so we shall not restrict ourselves to strong observables and will consider instead weak observables in what follows. Note that when reducing the theory to the space $\hat{\Gamma}$, both the observables and their HVF can be projected down unambiguously to $\hat{\Gamma}$.

Let us now explore what this characterization of observables implies. First, note that equation (6) is also telling us that the change of f along the gauge vector fields X_i^a is zero. This means that an observable O is a function f that is invariant along the gauge orbits. Given that we should only consider such functions in the description of the physical system, one has to conclude that the points on the gauge orbit have to be indistinguishable. Otherwise, one would be able to find a function that could separate the points along an orbit, but then that function would fail to be an observable. Given that the physical equivalence or not of points on the constrained surface is given by means of the observables themselves, it is easy to see that the usual practice of regarding such points as physically equivalent is fully justified².

Let us now consider the so called *Master Constraint* \mathbf{M} [5]. The idea is to define a single function, whose vanishing is equivalent to the vanishing of all the constraints. The simplest is to consider a positive quadratic form K^{ij} and take,

$$\mathbf{M} := K^{ij} C_i C_j = 0, \quad (7)$$

as the new condition. Clearly $\mathbf{M} = 0$ iff $C_i = 0$ for all i , so it defines the same subspace of Γ . However note that it represents an *inadmissible description* of $\bar{\Gamma}$ [2] given that its gradient $\nabla_a \mathbf{M}$ vanishes everywhere on $\bar{\Gamma}$ and its HVF also vanishes on $\bar{\Gamma}$ and therefore it does not ‘generate’ anything.

What happens then to the observables? If one took naively the condition (6), with \mathbf{M} replacing C_i as a criteria to determine when a function is an observable, then one would not conclude much given that *any* function f satisfies

$$0 = X_{\mathbf{M}}^a \nabla_a f = -X_f^a \nabla_a \mathbf{M}, \quad (8)$$

for the trivial reason that $\nabla_a \mathbf{M}$ (and $X_{\mathbf{M}}^a$) vanishes exactly at $\bar{\Gamma}$. Instead one should ask, as before, that the observables preserve the constraint surface. This means that the finite symplectomorphism generated by f should preserve \mathbf{M} and thus $\bar{\Gamma}$. This condition can be written, in terms of n -Poisson brackets $\{\cdot, \cdot\}_{(n)}$ as [5]:

$$\alpha_t^f[g] := e^{t\mathcal{L}_{X_f}} \cdot g := \sum_{n=0}^{\infty} \frac{t^n}{n!} \{g, f\}_{(n)} \quad (9)$$

² Note that this geometric characterization of observables is somewhat parallel to the algebraic characterization detailed in [2] which focuses on preserving the algebraic properties of the ideal of observables.

where $\{g, f\}_{(n+1)} := \{\{g, f\}_{(n)}, f\}$ and $\{g, f\}_{(0)} = f$. If we now apply it to \mathbf{M} we see that the condition

$$\alpha_t^f[\mathbf{M}]|_{\bar{\Gamma}} = 0 \quad (10)$$

which physically asks that f preserves $\bar{\Gamma}$ (and is thus an observable), is equivalent to.

$$\{\mathbf{M}, f\}_{(n)} = 0 \quad (11)$$

for all n , when evaluated on $\bar{\Gamma}$. The first condition, namely for $n = 1$, given by $\{\mathbf{M}, f\}_{(1)} = \{\mathbf{M}, f\} = 0$ is always satisfied on $\bar{\Gamma}$ (as we have seen before). Thus the first non-trivial condition on the function to be an observable is:

$$0 = \{\mathbf{M}, f\}_{(2)} = \{\{\mathbf{M}, f\}, f\} \quad (12)$$

which is the condition introduced in [5] as the ‘Master Equation’. As we have seen here this condition is a natural consequence of the requirement that finite symplectomorphisms generated by an observable leave $\bar{\Gamma}$ invariant.

This concludes our brief description of the classical theory. Let us now consider the quantum theory.

III. QUANTUM CONSTRAINED SYSTEMS

This section has two parts. In the first one, we give a review of the geometrical formulation of quantum mechanics. In the second part, we put forward its extension to deal with constrained systems. We study the properties of observables and their algebraic properties.

A. Geometric Quantum Mechanics

Let us recall the geometrical formalism of quantum mechanics. This fascinating subject has been ‘re-discovered’ several times during the past decades. For an incomplete list of references see [7].

For simplicity in our presentation we shall restrict our discussion to systems with a finite dimensional Hilbert space. The generalization to the infinite dimensional case is straightforward [7]. Denote by \mathcal{P} the space of rays in the Hilbert space \mathcal{H} . That is, given two states $|\phi\rangle$ and $|\psi\rangle$ in \mathcal{H} such that they are proportional $|\psi\rangle = \alpha|\phi\rangle$ for $\alpha \in \mathbb{C}$, one regards the two states as equivalent and, therefore, both vectors belong to the same equivalence class $[|\psi\rangle] \in \mathcal{P}$. In the finite dimensional case \mathcal{P} will be the complex projective space $\mathbb{C}P^{n-1}$, since \mathcal{H} can be identified with \mathbb{C}^n .

It is convenient to view \mathcal{H} as a *real* vector space equipped with a complex structure (recall that a complex structure J is a linear mapping $J : \mathcal{H} \rightarrow \mathcal{H}$ such that $J^2 = -1$). Let us decompose the Hermitian inner product into real and imaginary parts,

$$\langle \Psi | \Phi \rangle = G(\Psi, \Phi) - i\Omega(\Psi, \Phi), \quad (13)$$

where G is a Riemannian inner product on \mathcal{H} and Ω is a symplectic form.

Let us restrict our attention to the sphere S of normalized states. The true space of states is given by the quotient of S by the $U(1)$ action of states that differ by a ‘phase’, i.e. the projective space \mathcal{P} . The complex structure J is the generator of the $U(1)$ action (J plays

the role of the imaginary unit i when the Hilbert space is taken to be real). Since the phase rotations preserve the norm of the states, both the real and imaginary parts of the inner product can be projected down to \mathcal{P} .

Therefore, the structure on \mathcal{P} which is induced by the Hermitian inner product is given by a Riemannian metric g and a symplectic two-form Ω . The pair (g, Ω) defines a Kähler structure on \mathcal{P} (Recall that a Kähler structure is a triplet (M, g, Ω) where M is a complex manifold (with complex structure J), g is a Riemannian metric and Ω is a symplectic two-form, such that they are compatible with the complex structure).

The space \mathcal{P} of quantum states has then the structure of a Kähler manifold, so, in particular, it is a symplectic manifold and can be regarded as a ‘phase space’ by itself. It turns out that the quantum dynamics can be described by a ‘classical dynamics’, that is, with the same symplectic description that is used for classical mechanics. Let us see how it works. In quantum mechanics, Hermitian operators on \mathcal{H} are generators of unitary transformations (through exponentiation) whereas in classical mechanics, generators of canonical transformations are real valued functions $f : \mathcal{P} \rightarrow \mathbb{R}$. We would like then to associate with each operator F on \mathcal{H} a function f on \mathcal{P} . There is a natural candidate for such function: $f := \langle F \rangle_S$ (denote it by $f = \langle F \rangle$). The Hamiltonian vector field X_f of such a function is a Killing field of the Riemannian metric g . The converse also holds, so there is a one to one correspondence between self-adjoint operators on \mathcal{H} and real valued functions (‘quantum observables’) on \mathcal{P} whose Hamiltonian vector fields are symmetries of the Kähler structure.

There is also a simple relation between a natural vector field on \mathcal{H} generated by F and the Hamiltonian vector field associated to f on \mathcal{P} . Consider on S a ‘point’ ψ and an operator F on \mathcal{H} . Define the vector $X_F|_\psi := \frac{d}{dt} \exp[-JFt]\psi|_{t=0} = -JF\psi$. This is the generator of a one parameter family (labeled by t) of unitary transformation on \mathcal{H} . Therefore, it preserves the Hermitian inner-product. The key result is that X_F projects down to \mathcal{P} and the projection is precisely the Hamiltonian vector field X_f of f on the symplectic manifold (\mathcal{P}, Ω) .

Dynamical evolution is generated by the Hamiltonian vector field X_h when we choose as our observable the Hamiltonian $h = \langle H \rangle$. Thus, Schrödinger evolution is described by Hamiltonian dynamics, exactly as in classical mechanics.

One can define the Poisson bracket between a pair of observables (f, g) from the inverse of the symplectic two form Ω^{ab} ,

$$\{f, g\} := \Omega(X_g, X_f) = \Omega^{ab}(\partial_a f)(\partial_b g). \quad (14)$$

The Poisson bracket is well defined for arbitrary functions on \mathcal{P} , but when restricted to observables, we have,

$$\langle -i[F, G] \rangle = \{f, g\}. \quad (15)$$

This is in fact a slight generalization of Ehrenfest theorem, since when we consider the ‘time evolution’ of the observable f we have the Poisson bracket $\{f, h\} = \dot{f}$,

$$\dot{f} = \langle -i[F, H] \rangle. \quad (16)$$

As we have seen, the symplectic aspect of the quantum state space is completely analogous to classical mechanics. Notice that, since only those functions whose Hamiltonian vector fields preserve the metric are regarded as ‘quantum observables’ on \mathcal{P} , they represent a very small subset of the set of functions on \mathcal{P} .

Let us now explore the another facet of the quantum state space \mathcal{P} that is absent in classical mechanics: Riemannian geometry defined by g . Roughly speaking, the information

contained in the metric g has to do with those features which are unique to the quantum realm, namely, those related to measurement and ‘probabilities’. We can define a Riemannian product (f, h) between two observables as

$$(f, h) := g(X_f, X_h) = g^{ab}(\partial_a f)(\partial_b h). \quad (17)$$

This product has a very direct physical interpretation in terms of the dispersion of the operator in the given state:

$$(f, f) = 2(\Delta F)^2. \quad (18)$$

Therefore, the length of X_f is the uncertainty of the observable F .

The metric g has also an important role in those issues related to measurements. Note that eigenvectors of the Hermitian operator F associated to the quantum observable f correspond to points ϕ_i in \mathcal{P} at which f has local extrema. These points correspond to zeros of the Hamiltonian vector field X_f , and the eigenvalues f_i are the values of the observable $f_i = f(\phi_i)$ at these points.

If the system is in the state Ψ , what are the probabilities of measuring the eigenvalues f_i ? The answer is strikingly simple: measure the geodesic distance given by g from the point Ψ to the point ϕ_i (denote it by $d(\Psi, \phi_i)$). The probability of measuring f_i is then,

$$P_i(\Psi) = \cos^2 [d(\Psi, \phi_i)]. \quad (19)$$

Therefore, a state Ψ is more likely to ‘collapse’ to a nearby state than to a distant one when a measurement is performed. This ends our brief review of the geometric formulation of quantum mechanics.

B. Quantum Constraints

In this section we will consider an extension of the geometric description for quantum constrained systems. We shall for the moment restrict our attention to the case of a single constraint and consider the more general case later. The objective in this part is to put forward a proposal for imposing the ‘Dirac condition’ on quantum states within the geometrical formulation described in the last part. In particular, the objective is to translate the condition

$$\hat{C} \cdot \Psi = 0, \quad (20)$$

into the language of ‘quantum observables’ and hamiltonian vector fields that are also used in the geometrical description. (Note that an alternative, equivalent, condition for Ψ is given by the condition $e^{i\hat{C}} \cdot \Psi = \Psi$.) The most naive condition for implementing the constraint, namely asking that the expectation value of \hat{C} (which will be assumed to be self-adjoint on the kinematical Hilbert space) vanishes,

$$\langle \Psi | \hat{C} | \Psi \rangle = 0$$

has the problem of being too weak, since there are many states for which the expectation value vanishes, but such that $\hat{C} \cdot \Psi \neq 0$. It is then natural to consider instead the following condition

$$\langle \Psi | \hat{C}^2 | \Psi \rangle = 0. \quad (21)$$

If the operator \hat{C}^2 is indeed positive (which will be the case if \hat{C} is self-adjoint), then the condition (21) is equivalent to (20) since $\langle \Psi | \hat{C}^2 | \Psi \rangle = |\hat{C} | \Psi \rangle|^2 = 0 \Leftrightarrow \hat{C} | \Psi \rangle = 0$. Note that this condition is meaningful only when zero is a discrete point in the spectrum of \hat{C} . Thus, the function $\mathcal{C} := \overline{\mathcal{C}^2} = \langle \Psi | \hat{C}^2 | \Psi \rangle$ on \mathcal{P} is precisely the quantum equivalent of the classical constraint function and the condition (21) is the analogue of the classical $C = 0$ condition. Clearly, the function \mathcal{C} is different from the function $c^2 = |\langle \Psi | \hat{C} | \Psi \rangle|^2$ on \mathcal{P} . It is interesting to note that we can also implement the condition $e^{i\hat{C}} \Psi = \Psi$ in the geometric language by requiring: $\langle (e^{i\hat{C}} - 1)^\dagger (e^{i\hat{C}} - 1) \rangle = 0$. This yields,

$$\langle \Psi | (1 - \cos(\hat{C})) | \Psi \rangle = 0, \quad (22)$$

which involves the simultaneous vanishing of the expectation values for all even powers of the quantum constraint \hat{C} .³

Let us now explore the consequences of the condition (21) that defines the physical state space $\mathcal{P}_{\text{phy}} \subset \mathcal{P}$. Just as in the classical theory the physical state space is defined as a submanifold of the state space \mathcal{P} , where the function \mathcal{C} takes a constant value. One might wonder then whether the symplectic structure Ω is also degenerate along the gauge orbits of \mathcal{C} and whether one has to reduce along those ‘gauge directions’. The geometric setting we have encountered seems to suggest this scenario that goes, however, against the common wisdom that the quantum reduction imposed by (21) is enough. Let us further explore the issue to resolve this apparent tension.

Recall that the Hamiltonian vector field of an operator \hat{F} , at the point Ψ , is given by the (projection to \mathcal{P} of the) vector $-J F \Psi$. In the case of the operator \hat{C} , its Hamiltonian vector field vanishes exactly on the physical Hilbert space (and \mathcal{P}_{phy}) given that $X_C|_\Psi = -J \hat{C} \Psi = 0$. Thus, the constraint function $\bar{\mathcal{C}}^2$ (and also $c = \langle \hat{C} \rangle$) does not generate anything on \mathcal{P}_{phy} . Thus, in contrast with the classical scenario, there are no degenerate directions of the symplectic structure associated to the constraint. This answers the question posed above.

In particular, another common apparent tension becomes clarified with our previous discussion. It is somewhat natural to regard the orbit $e^{i\lambda\hat{C}} \cdot \Psi$ of Ψ on \mathcal{P} as the equivalent of the gauge orbits generated by the constraint on $\bar{\Gamma}$. This expectation is motivated by the fact that the group averaging construction [3] uses this ‘gauge orbit’ and averages over its states to construct a solution to the constraint equation. Any two points along the orbit yield the same physical state and are thus, in a sense, equivalent. This is similar to the process of averaging functions along classical gauge orbits to obtain physical observables. But it is clear that this is only an approximate analogy. In the classical theory any point of the orbit is a physically admissible configuration, since it satisfies all the constraints, so the equivalence class defined by the orbit that projects to a physical state is made out of admissible configurations. This is not the case in the quantum ‘gauge orbit’. Unless it lies on the kernel, a generic state in that orbit is not physical. The group average procedure is adding vectors, so the average yields a vector that does not belong to the orbit; it is a true projection mapping η within the space \mathcal{P} from the ‘gauge orbit’ to a different point not belonging to it. Clearly, if we start with a solution to the constraints, then the orbit is trivial and the group average yields the same point. Thus, it is important to recognize

³ Note that this does not impose any new condition on the states. If they already satisfy (21), then $\langle \Psi | \hat{C}^4 | \Psi \rangle = \langle \Psi | \hat{C} \hat{C}^2 \hat{C} | \Psi \rangle = 0$, and similarly for higher powers.

the fundamental difference between the classical projection from $\bar{\Gamma}$ to $\hat{\Gamma}$ and the quantum projection from \mathcal{P} to \mathcal{P}_{phy} . Both involve an equivalence class and the quotient by the orbits. The difference is that in the classical case, the physics (as seen by the true observables) is the same for any element of the equivalence class, so it is rather natural to identify them as ‘the same’ state. In the quantum case, the elements of the orbit contain in a sense the same information but it is only after the true projection as defined by the group average mapping η that the physical state arises. None of the elements of the orbit are, *per se*, physical states. This difference tells us that the physical quantum state space \mathcal{P}_{phy} involves a different type of quotient of \mathcal{P} by the ‘quantum gauge orbits’, than one might have expected by taking the analogy with the classical scenario too seriously.

Let us now consider observables. The question of when an operator \hat{F} is a physical observable follows a similar path as in the classical theory. Recall that in that case we required that an observable O is a function of phase space such that the one parameter family of symplectomorphisms it generates leaves the constrained surface invariant. The corresponding criteria in the quantum theory is to require that the one parameter family of unitary transformations a physical observable \hat{O} generates leaves the quantum state space \mathcal{P}_{phy} invariant. This means that the one parameter family of states

$$\Phi(\lambda) := e^{i\lambda\hat{O}} \cdot \Psi_{\text{phy}}, \quad (23)$$

for all λ and $\Psi_{\text{phy}} \in \mathcal{P}_{\text{phy}}$, must also be a physical state. Namely, it must satisfy

$$\langle \Phi(\lambda) | \hat{C}^2 | \Phi(\lambda) \rangle = 0 \quad (24)$$

for all λ . This can be rewritten as,

$$\langle \Psi_{\text{phy}} | \hat{C}^2 - i\lambda[\hat{O}, \hat{C}^2] + \frac{\lambda^2}{2} [\hat{O}, [\hat{O}, \hat{C}^2]] + \dots | \Psi_{\text{phy}} \rangle = 0 \quad (25)$$

This means that the operator

$$e^{-i\lambda\hat{O}} \hat{C}^2 e^{i\lambda\hat{O}} = \sum_{n=0}^{\infty} \frac{(-i\lambda)^n}{n!} [\hat{O}, \hat{C}^2]_{(n)}$$

with $[\hat{O}, \hat{C}^2]_{(0)} = \hat{C}^2$ and $[\hat{O}, \hat{C}^2]_{(n+1)} = [\hat{O}, [\hat{O}, \hat{C}^2]_{(n)}]$, must have vanishing expectation values on any physical state. It is easy to see that the first non-trivial constraint on the observable \hat{O} is the condition $\langle \Psi_{\text{phy}} | [\hat{O}, [\hat{O}, \hat{C}^2]] | \Psi_{\text{phy}} \rangle = 0$. This in turn is satisfied if and only if,

$$\langle \Psi_{\text{phy}} | \hat{O} \hat{C}^2 \hat{O} | \Psi_{\text{phy}} \rangle = 0 \quad (26)$$

which tells us that: i) The state $\hat{O} | \Psi_{\text{phy}} \rangle$ is also physical, ii) the Hamiltonian vector field $X_{\hat{O}} = -J\hat{O}\Psi$ (and its projection) is tangent to \mathcal{P}_{phy} ; iii) The condition on the function $\langle \hat{O} \rangle$ is that its n -Poisson brackets with \bar{C}^2 vanish. Note also that we have arrived to the quantum analogue of the double commutator condition of the master constraint program [5], *as if* we had ‘quantized’ the classical condition (12) with $\hat{\mathbf{M}} = \hat{C}^2$. We have not. We have simply restated the Dirac condition (20) in terms of expectation values and we have implemented the natural condition for physical observables in terms of their invariance properties. Note that if we have more than one constraint, we will have to impose a condition

for each constraint, or a linear combination generated by a positive quadratic form, but the discussion is unchanged for each one of them. We now end this section with several remarks.

Constraint Algebra: In the classical theory a set of first class constraints C_i satisfy, on the whole phase space Γ , the relations:

$$\{C_i, C_j\} = F_{ij}^k C_k \quad (27)$$

These relations can be translated to a commutator of their Hamiltonian vector fields

$$[X_i, X_j] = -X_{F_{ij}^k C_k}, \quad (28)$$

which is closed when one is restricted to $\bar{\Gamma}$: $[X_i, X_j]|_{\bar{\Gamma}} = F_{ij}^k X_{C_k}$. Thus, the relation between Poisson brackets and vector fields for the constraints is only satisfied on the constrained surface $\bar{\Gamma}$. As we have noted before, this algebraic relations between constraint functions/vector fields on the constraint surface carries the information that the HVF of the constraint functions are all tangent to $\bar{\Gamma}$. The precise algebraic relation (i.e. the structure functions F_{ij}^k) does not seem to be fundamental, since one can always find suitable ‘Darboux coordinates’ that make the vector fields commute [2]. Furthermore, when we go to the quotient space, the reduced phase space $\hat{\Gamma}$, the projection of the vector fields X_i^a to $\hat{\Gamma}$ vanish for all i . Thus, on the physically relevant phase space $\hat{\Gamma}$, the constraints do not ‘generate anything’. The quantum physical state space \mathcal{P}_{phy} is the corresponding object in the quantum theory. In both $\hat{\Gamma}$ and \mathcal{P}_{phy} , the ‘constraint algebra’ becomes irrelevant. Furthermore, if one assumes that one has a quantum theory that implements the constraints (that could have been obtained by quantizing the reduced phase space or via the Dirac procedure), in the classical limit one expects to recover the reduced phase space $\hat{\Gamma}$ and not the constraint surface $\bar{\Gamma}$ where the ‘Dirac algebra’ is well defined [9]. This is part of the well know problem of the ‘frozen formalism’ and the recovery of dynamics for totally constrained systems [1, 10].

Master Constraint. The Master Constraint Program as put forward by Thiemann has several objectives. In particular it has been argued that it might be technically easier to impose a constraint of the form $\mathbf{M} \cdot \Psi = 0$, than several constraints, in particular for field theories such as general relativity. We have no particular comments on this possibilities. What we have shown here is that the apparent difficulties in the constraint algebra and the so-called ‘Master Equation’ do not arise and that, rather, they are rather natural from the standard Dirac procedure, when analyzed from the geometric perspective⁴.

Off-shell algebra. It is not uncommon to see the statement that the off-shell closure of the constraint algebra is important for removing possible *gauge* anomalies. Let us now see what the geometric formulation tells us regarding the off-shell algebra of the constraints. The natural objects to consider in this case are the vector fields $X_{C_i} = X_{\overline{C^2}_i}$ that correspond to the functions defining the physical state space \mathcal{P}_{phy} (by requiring the vanishing of all C_i).

⁴ Sometimes it is also argued that instead of the condition $\hat{\mathbf{M}} = 0$, that might not have a solution in the quantum theory, one can have $\hat{\mathbf{M}} - \delta = 0$ for some small (in classical scales) quantity δ . This condition now reads, in the geometric language as $\mathcal{C} - \delta = 0$. That is, the quantum constraint condition is again slightly shifted, but all the geometry, including the relevant vector fields and commutators remain invariant.

The commutator of two such fields is given by

$$[X_{\bar{C}_i^2}, X_{\bar{C}_j^2}] = X_{\langle \hat{C}_i^2, \hat{C}_j^2 \rangle} \quad (29)$$

Thus, within the geometric formulation, the relevant quantities in order to compute the commutator of vector fields are the commutators of the *squares* of the constraint operators $[\hat{C}_i^2, \hat{C}_j^2]$. This has to be contrasted to the standard treatment where the relevant object are taken to be the commutator between the constraints themselves. Of course, all the constraint vector fields and their commutators vanish on-shell, that is on the submanifold \mathcal{P}_{phy} . When we consider observables \hat{O} , the relevant quantity for the geometric formulation is again the Poisson bracket defined by Ω , which contains information regarding the commutator of the vector fields corresponding to the observable \hat{O} and \hat{C}_i^2 (which in turn is obtained from $[\hat{C}_i^2, \hat{O}]$). Needless to say, this matter needs to be further studied.

IV. DISCUSSION

In this note we have addressed the issue of imposing the quantum constraints within the Dirac-Bergmann approach to constrained quantization. We have recast this problem within the geometric formulation of quantum mechanics, and have shown that the condition that the states be annihilated when acted upon by the constraints, can be translated and put just as in the classical setting: by requiring the vanishing of a function (or set of functions) on the quantum state space. Just as in the classical case, the solution to this condition is a submanifold of the space of kinematical states. The function that implements this condition in the quantum state space is the expectation value of the square of the constraint (or the sum of squares for more than one constraint). The main difference between the classical and the quantum cases is that the classical constrained surface has degenerate directions on the constraint surface that correspond to the gauge directions. Full reduction implies taking a quotient along the orbits. In the quantum case, there are no degenerate directions associated to the constraints and no further reduction is needed.

As we have seen, the requirement for general classical and quantum observables to become *physical* observables is that they preserve, under the motion they generate, the submanifold of physical states. This in turn implies that the condition on quantum observables is given by the double commutator with the *square* of the constraint(s) and thus, the contact with the master equation of the master constraint program arises in a natural fashion. The geometric formulation seems to suggest that the relevant quantities to consider when looking at the motions generated on the quantum state space are the squares of the constraints and not the constraints themselves. The motion generated by the unitary operators $e^{i\lambda\hat{C}}$ seems not to have the same fundamental role in the quantum theory of constrained systems when analyzed from the geometric perspective, as they have in the standard quantum theory without constraints. This could point to the conclusion that there is a fundamental difference between the motions generated by the constraints and those motions generated by observables of the theory, that might generate symmetries (i.e. as asymptotic Poincare generators, or canonical transformations generated by boundary terms). Thus, the possibility that there is a fundamental difference between possible *gauge* anomalies and regular (symmetry) anomalies deserves further attention.

In this article we have put forward a new perspective to look at quantum constrained systems. Even when the concrete conditions on states and observables that we have found

coincide with those of the standard treatment –not making the task of solving them any easier–, one can hope that this new viewpoint might shed some light on the still unresolved conceptual challenges that one faces when dealing with constrained systems and, in particular, in the construction of a quantum theory of gravity. It should be noted that we have considered the simplest possible scenario, namely the case in which the space of quantum physical states is a subspace of the kinematical one, that is realized when ‘zero’ lies in the discrete part of the spectrum. This condition is satisfied for only a few examples and many systems of interest do not possess this property. It is thus important to extend the current analysis to those more general cases. We shall leave that study for future investigations.

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